

Supporting Information

for

Oligoorganogermanes: interplay between aryl and trimethylsilyl substituents

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NMR Spectra of the Compounds Obtained

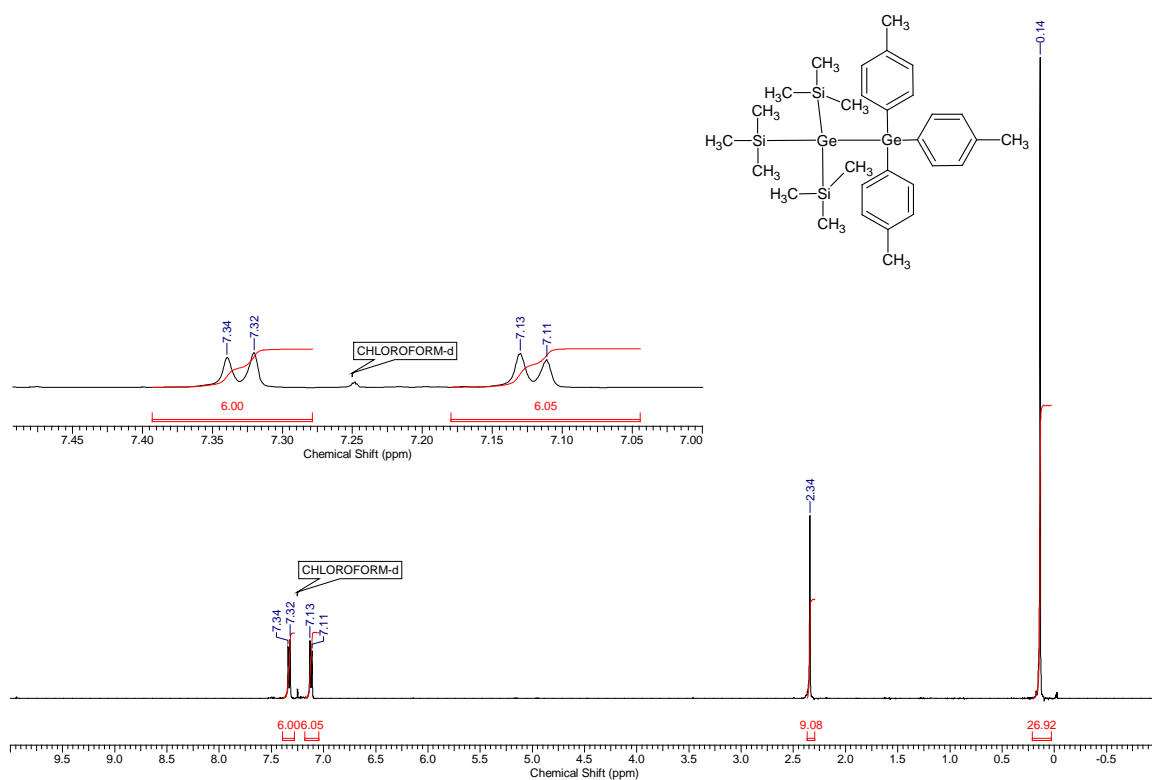


Fig. S1. ¹H NMR spectrum of $(\text{Me}_3\text{Si})_3\text{Ge}-\text{Ge}(\text{C}_6\text{H}_4\text{Me-}p)_3$ (1) (CDCl₃, RT).

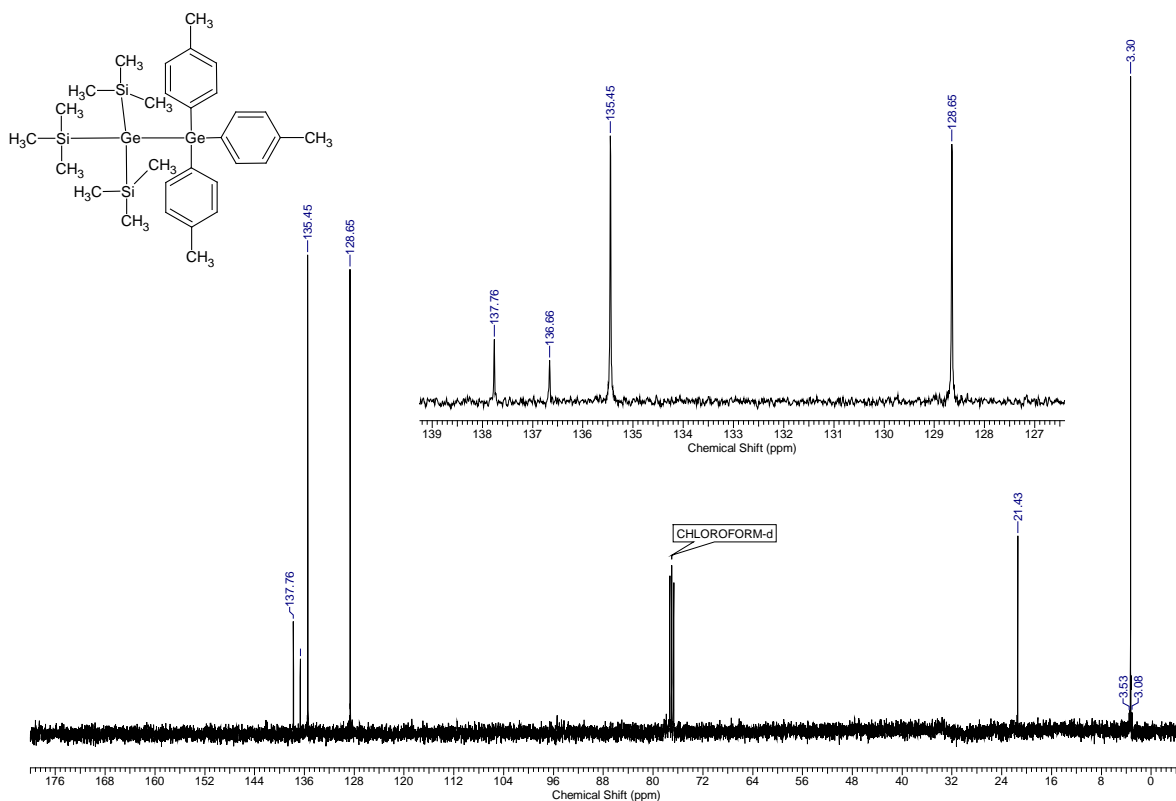


Fig. S2. ¹³C NMR spectrum of $(\text{Me}_3\text{Si})_3\text{Ge}-\text{Ge}(\text{C}_6\text{H}_4\text{Me-}p)_3$ (1) (CDCl₃, RT).

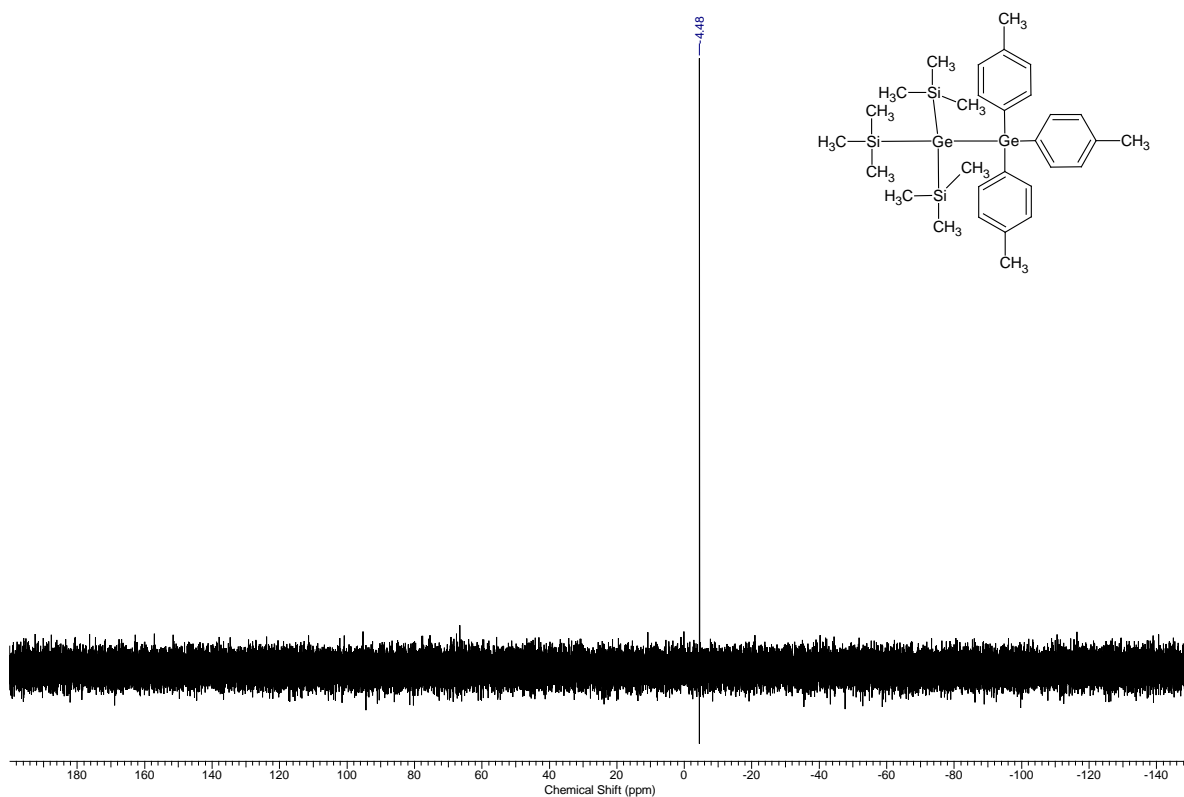


Fig. S3. ^{29}Si NMR spectrum of $(\text{Me}_3\text{Si})_3\text{Ge}-\text{Ge}(\text{C}_6\text{H}_4\text{Me-}p)_3$ (1) (CDCl_3 , RT).

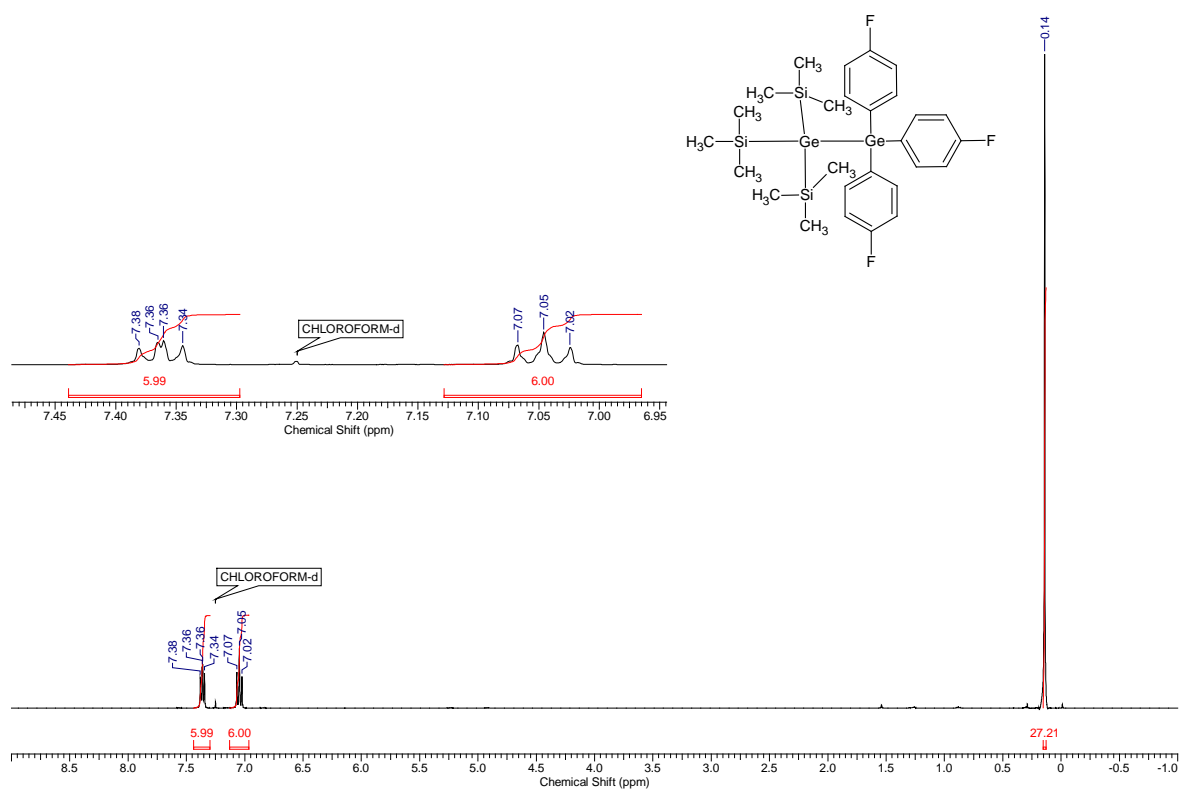


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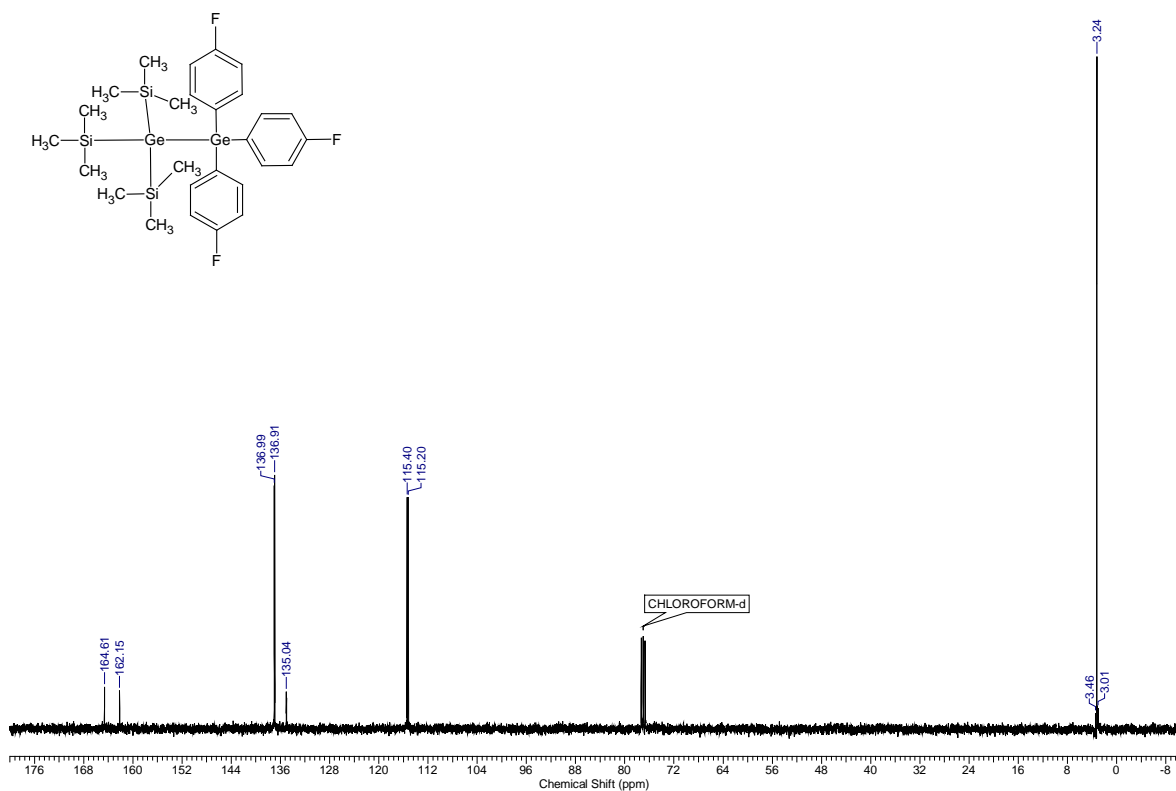


Fig. S5. ^{13}C NMR spectrum of $(\text{Me}_3\text{Si})_3\text{Ge}-\text{Ge}(\text{p-C}_6\text{H}_4\text{F})_3$ (2) (CDCl_3 , RT).

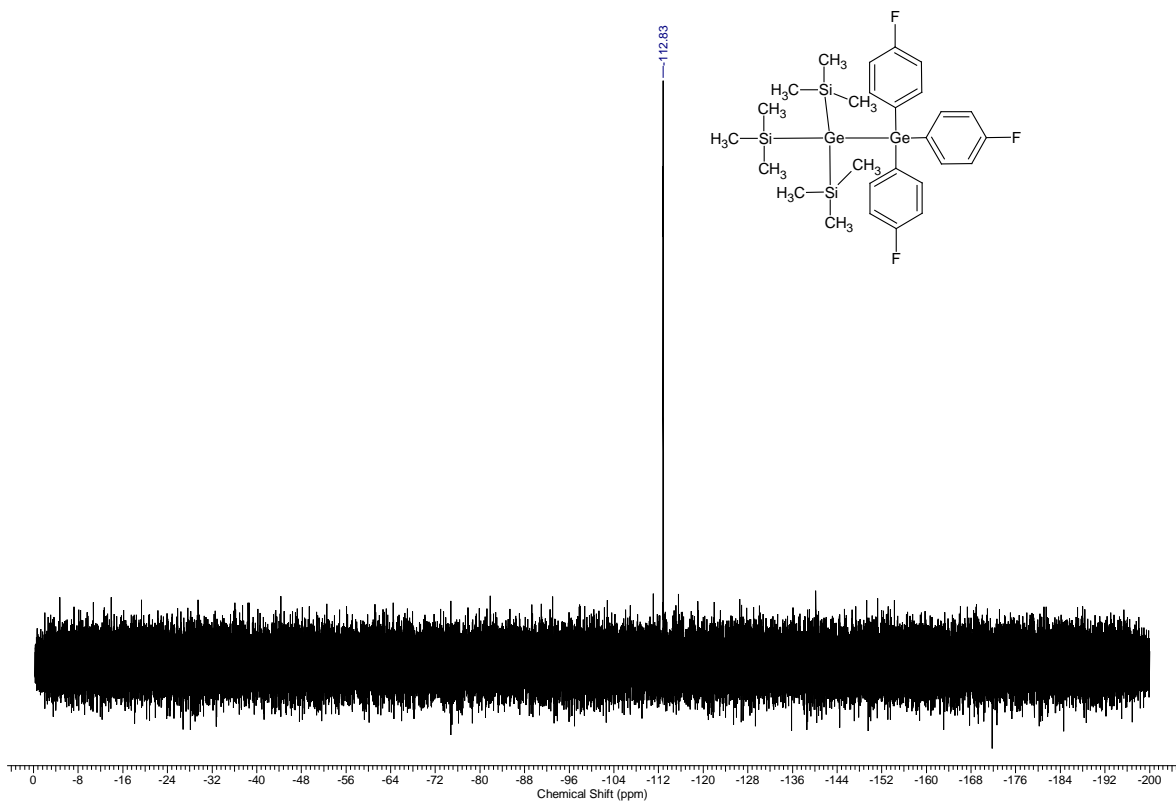


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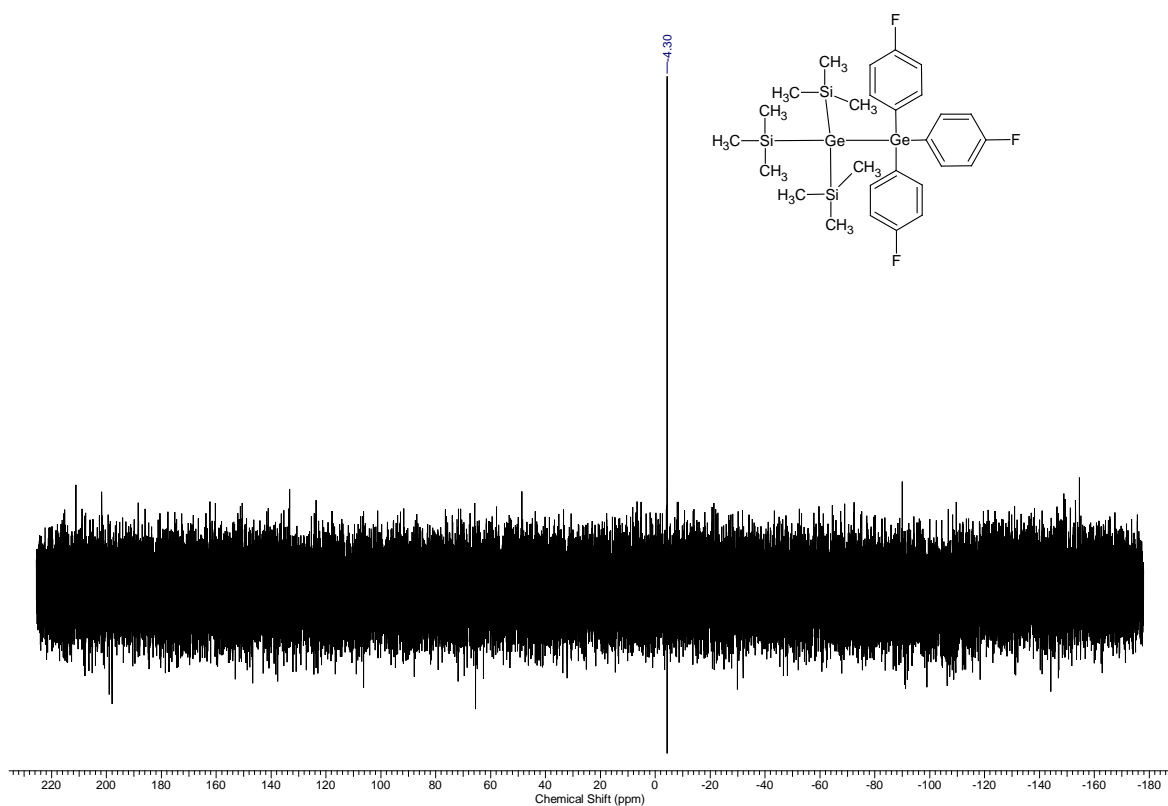


Fig. S7. ^{29}Si NMR spectrum of $(\text{Me}_3\text{Si})_3\text{Ge}-\text{Ge}(\text{p-C}_6\text{H}_4\text{F})_3$ (**2**) (CDCl_3 , RT).

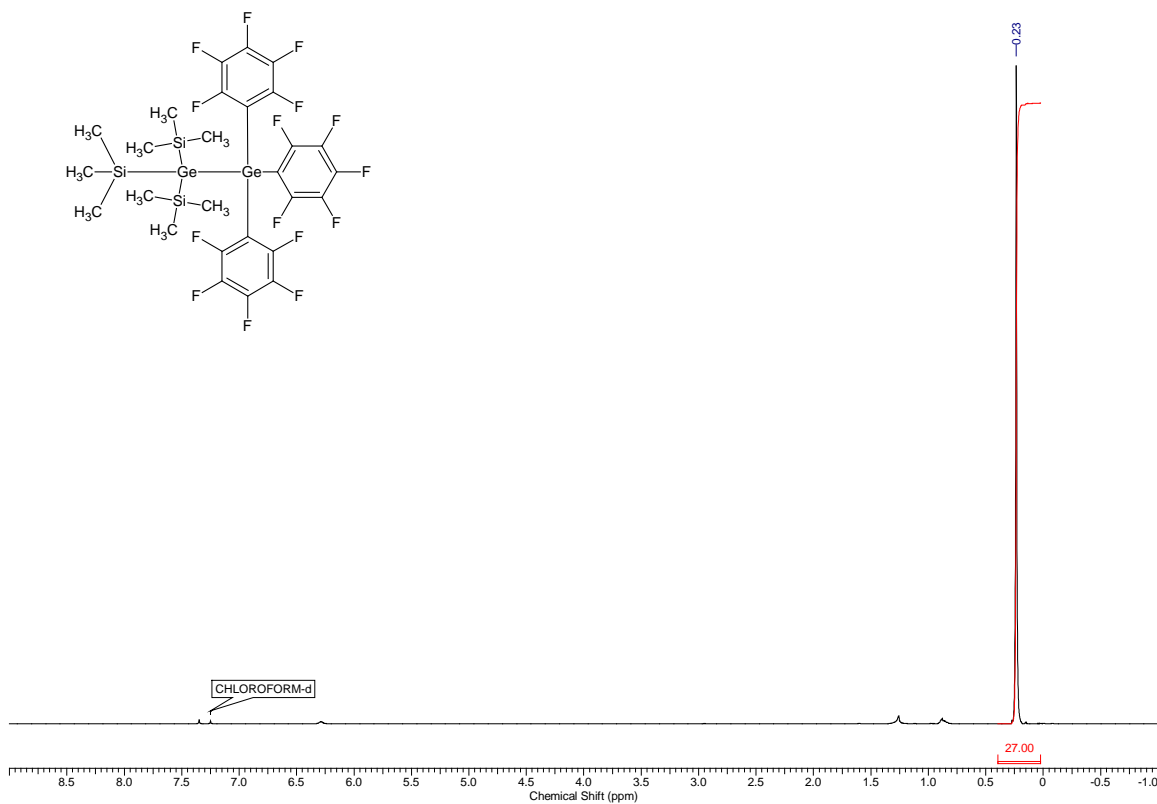


Fig. S8. ^1H NMR spectrum of $(\text{Me}_3\text{Si})_3\text{Ge}-\text{Ge}(\text{C}_6\text{F}_5)_3$ (**3**) (CDCl_3 , RT).

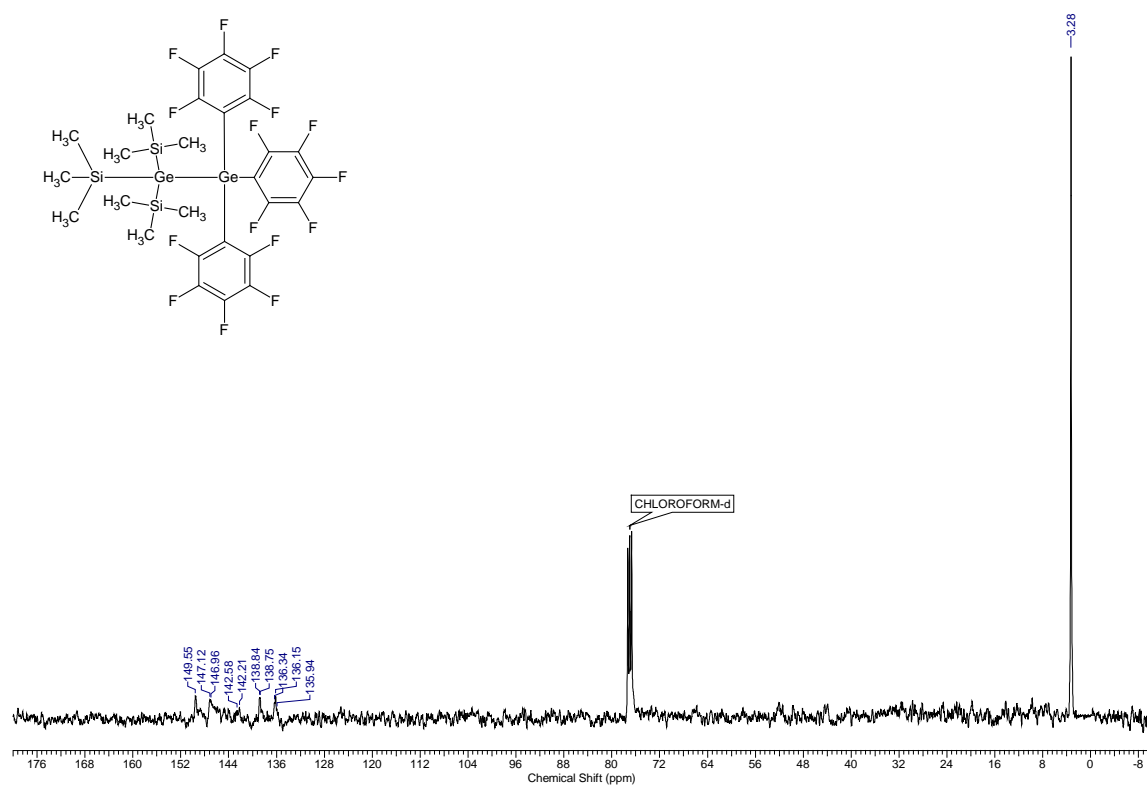


Fig. S9. ^{13}C NMR spectrum of $(\text{Me}_3\text{Si})_3\text{Ge}-\text{Ge}(\text{C}_6\text{F}_5)_3$ (3) (CDCl_3 , RT).

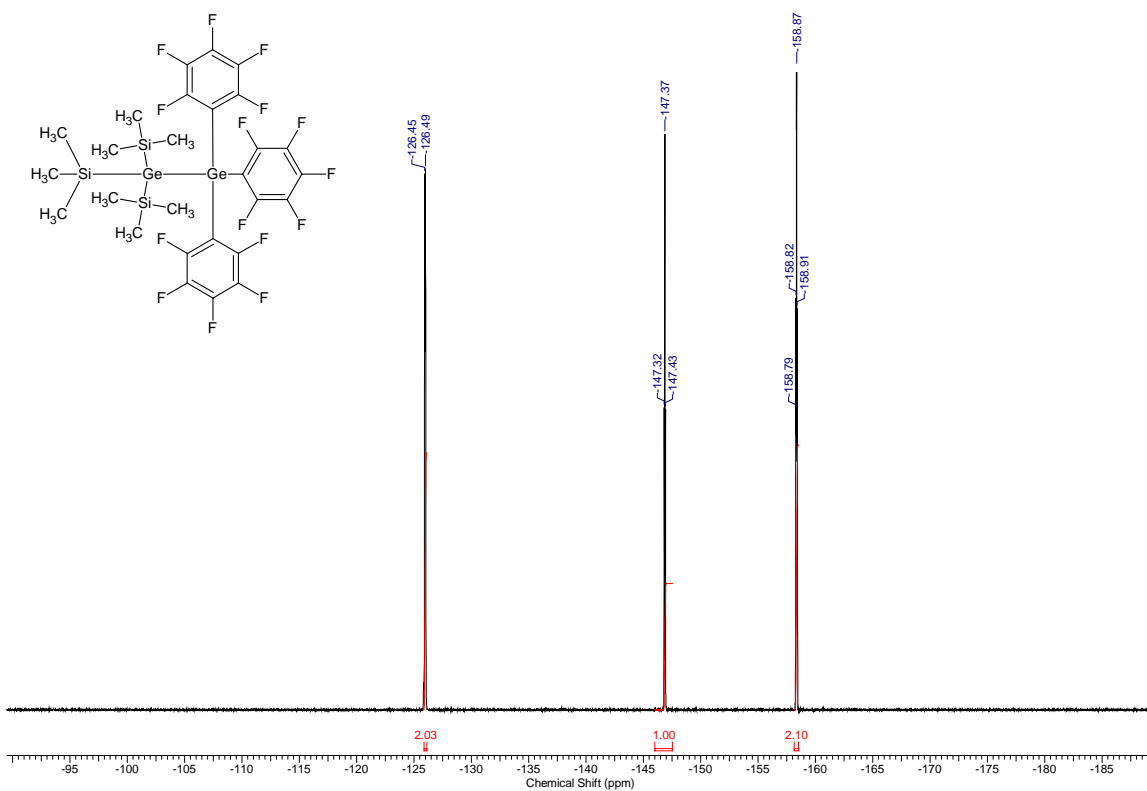


Fig. S10. ^{19}F NMR spectrum of $(\text{Me}_3\text{Si})_3\text{Ge}-\text{Ge}(\text{C}_6\text{F}_5)_3$ (3) (CDCl_3 , RT).

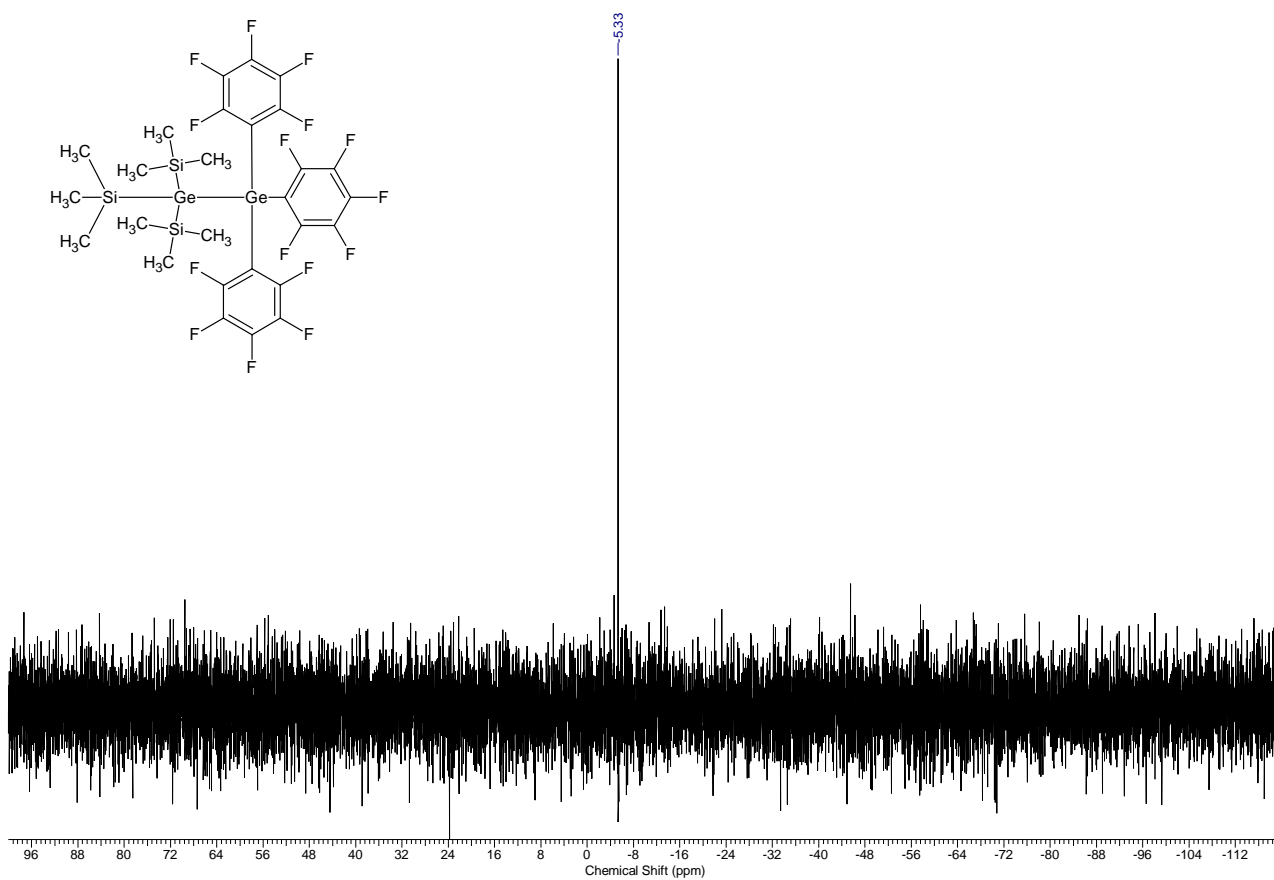
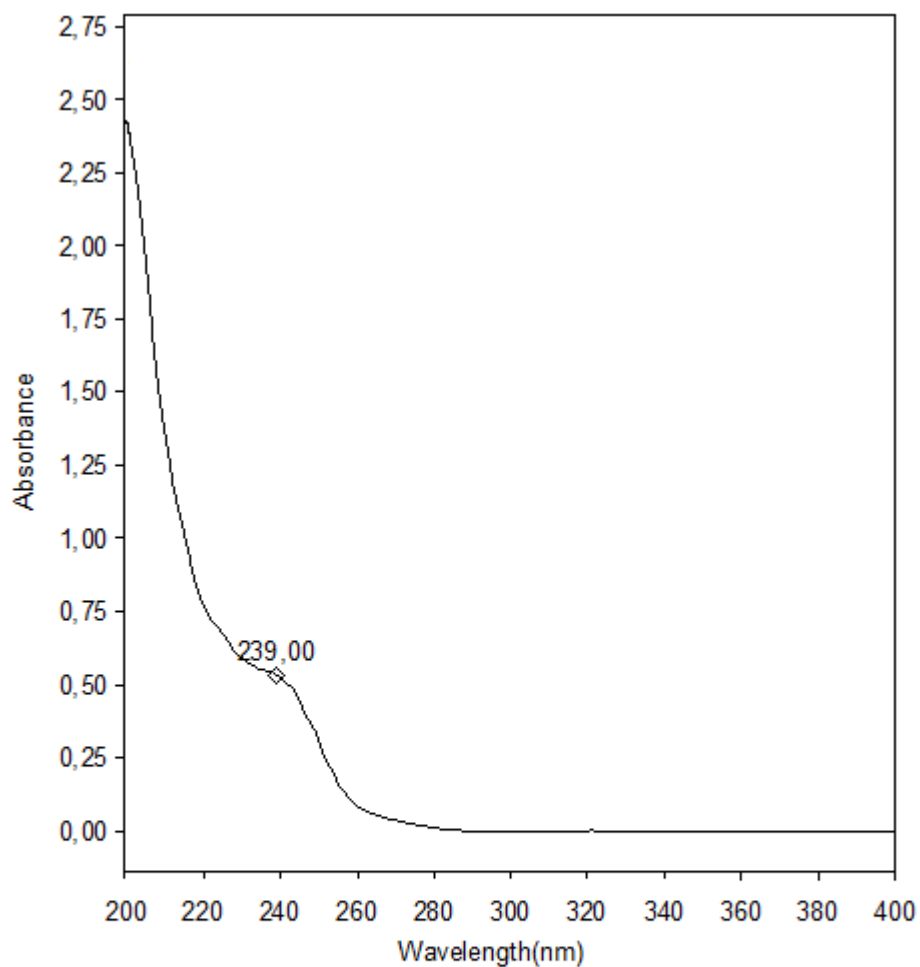


Fig. S11. ^{29}Si NMR spectrum of $(\text{Me}_3\text{Si})_3\text{Ge}-\text{Ge}(\text{C}_6\text{F}_5)_3$ (**3**) (CDCl_3 , RT).

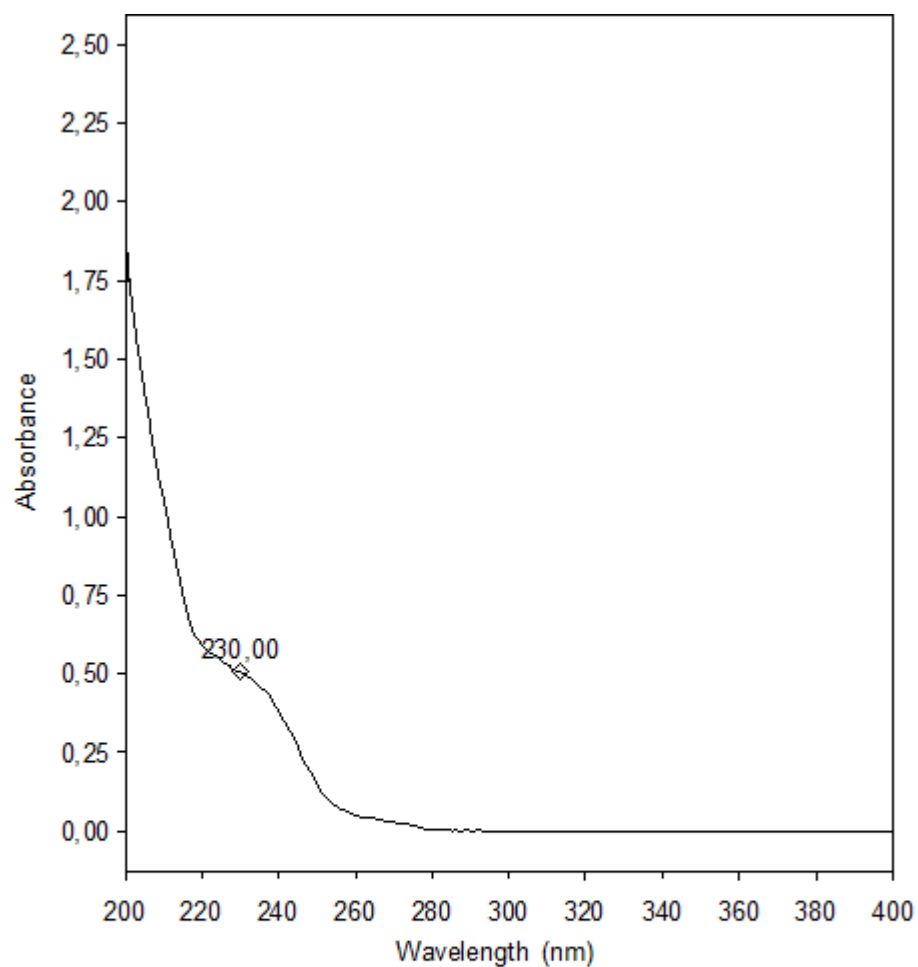
UV/vis Absorption Spectra of the Compounds Obtained



Batch : mar 4 C6H14 01 cm_03.sre

	A	B	C	D	E	F
1	mar 4 C6H14 01 c		1			
2	Cycle01	nm	239,00			
3	Manual	A	0,534			
4						
5						

Fig. S12. UV/vis Absorption Spectrum of $(\text{Me}_3\text{Si})_3\text{Ge-Ge}(\text{C}_6\text{H}_4\text{Me-}p)_3$ (**1**) (*n*-hexane, RT).



Batch : mar 5 C6H14 01 cm.sre

	A	B	C	D	E	F
1	mar 5 C6H14 01 c		1			
2	Cycle01	nm	230,00			
3	Manual	A	0,505			
4						
5						

Fig. S13. UV/vis Absorption Spectrum of $(\text{Me}_3\text{Si})_3\text{Ge-Ge}(p\text{-C}_6\text{H}_4\text{F})_3$ (**2**) (*n*-hexane, RT).

Data of the Single Crystal X-ray Diffraction Analysis

Table S1. Crystallographic data for complex (Me₃Si)₃Ge-Ge(C₆H₄Me-*p*)₃ (**1**) and (Me₃Si)₃Ge-Ge(C₆H₄F-*p*)₃ (**2**).

	(Me ₃ Si) ₃ Ge-Ge(C ₆ H ₄ Me- <i>p</i>) ₃ (1)	(Me ₃ Si) ₃ Ge-Ge(<i>p</i> -C ₆ H ₄ F) ₃ (2)
formula	C ₃₀ H ₄₈ Ge ₂ Si ₃	C ₂₇ H ₃₉ F ₃ Ge ₂ Si ₃
M_w	638.13	650.03
temperature (K)	150(2)	120(2)
size (mm)	0.25 x 0.20 x 0.06	0.24 x 0.20 x 0.18
crystal system	triclinic	triclinic
space group	<i>P</i> -1	<i>P</i> -1
<i>a</i> (Å)	10.3142(5)	12.6869(9)
<i>b</i> (Å)	12.5268(6)	16.0638(11)
<i>c</i> (Å)	14.3782(7)	16.0959(11)
α (deg)	92.799(1)	86.839(1)
β (deg)	99.352(1)	86.299(1)
γ (deg)	110.923(1)	81.912(1)
<i>V</i> (Å ³)	1700.61(14)	3237.4(4)
<i>Z</i>	2	4
P_{calcd} (g*cm ⁻³)	1.246	1.334
abs. coeff. μ (MoK α) (mm ⁻¹)	1.889	1.999
<i>F</i> (000)	668	1336
θ range (deg)	2.22 – 28.00	1.76 – 29.00
no. of collected/unique rflns.	17699 / 8197	36739 / 17152
R_{int}	0.0147	0.0202
data/restraints/parameters	8197 / 0 / 329	17152 / 0 / 649
goodness of fit on F^2	1.030	1.052
final <i>R</i> indices ($I > 2\sigma(I)$)	$R_1 = 0.0219,$ $wR_2 = 0.0583$	$R_1 = 0.0273,$ $wR_2 = 0.0630$
<i>R</i> indices (all data)	$R_1 = 0.0264,$ $wR_2 = 0.0603$	$R_1 = 0.0415,$ $wR_2 = 0.0671$
largest diff. peak/hole (e/Å ³)	-0.203 / 0.440	-0.285 / 0.377

Data of DFT calculations

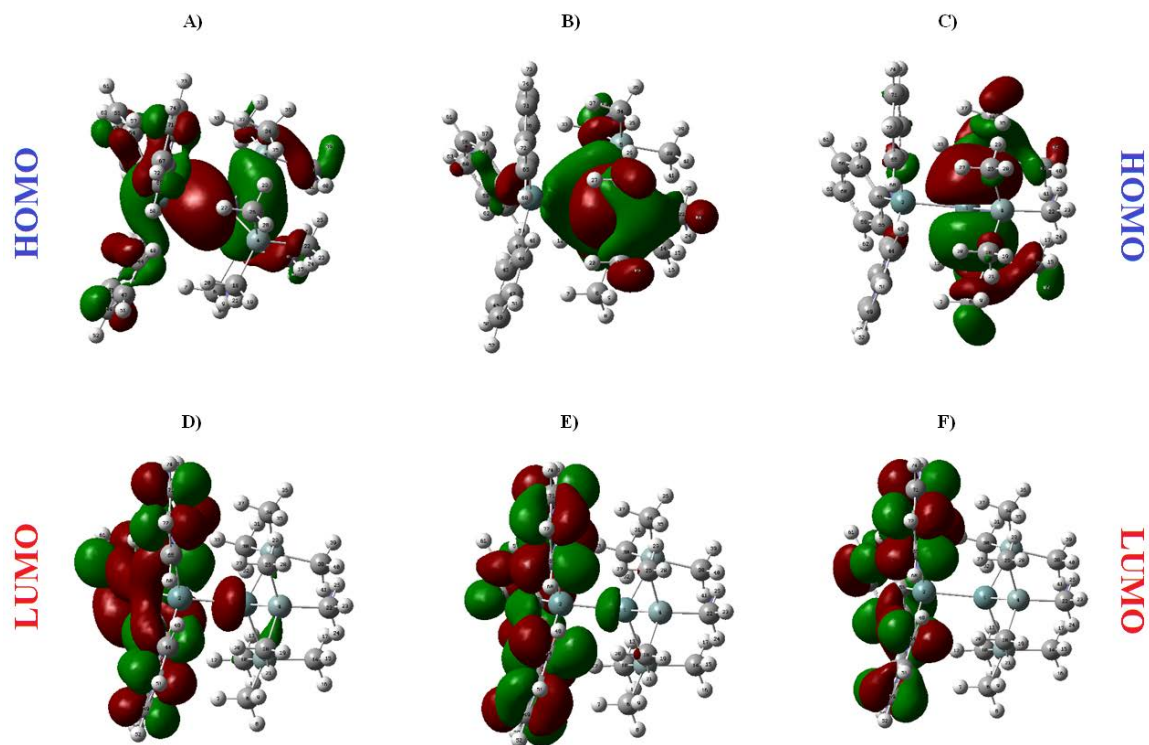


Fig. S14. Graphical representation of HOMO (A), HOMO-1 (B), HOMO-2 (C), LUMO (D), LUMO+1 (E), LUMO+2 (F) for compound (Me₃Si)₃Ge-GePh₃.